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COLLISIONAL EXCITATION OF NEON LIKE Ni XIX USING BREIT-PAULI R-MATRIX METHOD

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Abstract

Collision strength for the transition within the first five fine structure levels in Ni XIX are calculated using the Breit-Pauli R-matrix method. Configuration Interaction wave-functions are used to represent the target states included in the R-matrix expansion. The relativistic effects are incorporated in the Briet-Pauli approximation by including the one body mass-correction, Darwin, and spin orbit interaction terms in scattering equations. Our collision strengths are compared with those from other calculations. The collision strengths are integrated over a Maxwellian distribution of electron energies to obtain effective collision strengths over a wide temperature range.

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1 Introduction

In recent years there has been great interest in the study of neon-like ions due to their wide applications in numerous types of plasmas, including astrophysical plasma [1], magnetically-confined plasmas [2] and Z-pinch plasmas [3]. In the laser research concerning the soft X-ray region, Ne-like ions plays an important role in electron-collision excitation schemes and have been utilized successfully in the recent work by Nilson [4].

Several lines of Nickel ions have been observed in extreme ultraviolet (EUV) and ultraviolet (UV) solar flare spectra by the Solar Ultraviolet Measurements of Emitted Radiation (SUMER) spectrometer on the Solar and Heliospheric Observatory (SOHO). The $2s^2 2p^6\ ^3P_0 \rightarrow 2s^2 2p^5 3s\ ^3P_1$ line in Ni XIX have been identified by Feldman et al [5] in solar flare spectra. Accurate atomic data is needed for plasma diagnostics and also in the development of soft X-ray lasers. Zhang et al [6] have reported the fine structure collision strength in the Coulomb-Born exchange method for transitions from the ground state to n=3 levels of many neon-like ions including Ni XIX but no results have been reported, so far to our knowledge, for transitions within different fine structure levels.

In the present work we have used the Breit-Pauli R-matrix method [7,8] to calculate the collision strength including relativistic and resonance effects. The relativistic effects are included in the Breit-Pauli approximation [9,10,11] via one-body mass correction, Darwin and Spin-orbit interaction terms in scattering equations. We have considered the states $2s^2 2p^6\ ^1S^e$ and $2s^2 3p^5 3s\ (^1P^o, ^3P)$ of Ni XIX, which are represented by configuration interaction wave functions. Finally, the effective collision strengths are obtained by averaging the collision strengths over a Maxwellian distribution for the energy of the incident electron.

2 Target Calculation

The Configuration Interaction (CI) method has been used recently by Hibbert, Dourneuf, and Mohan[12] to calculate the wave functions for many ions of neon iso-electronic sequence using the CIV3 code. In the present scattering calculation, the LS states belonging to the ground $2s^2 2p^5(^1S)$ and $2s^2\ 2p^5\ 3s(^1P^0, ^3P^0)$ configurations are represented by restricted CI expansions, which includes most important configurations while keeping the scattering calculations tractable.

The wave functions are represented [13] by expansion of the form

$$\Phi(LS) = \sum_{i=0}^{M} a_i \phi_i(\alpha_i LS) \tag{1}$$

where each is constructed from one-electron orbitals whose angular momenta are coupled as specified by α_i to form total L and S common to M configurations. The radial part of each orbital is written as a linear combination of normalized Slater-type orbitals

$$P_{nl}(r) = \sum_{i=0}^{k} b_i \left(\frac{(2\zeta_i)^{2p_i+1}}{(2p_i)!}\right)^{1/2}\ r^{p_i} exp(-\zeta_i r) \tag{2}$$

The parameter b_i, ζ_i and p_i in equation (2) and the mixing coefficients a_i in equation (1) are determined variationally as described by Hibbert [14]. Here we have used seven orthogonal one-electron orbitals 1s, 2s, 2p, 3s, 3p, 3d, and 4d. The optimized parameters b_i, p_i and ζ_i for 3s, 3p, 3d and 4d orbitals are given in table 1. In table 2, we present the excitation thresholds, calculated with our fairly simple wave functions which agree reasonably well with the experimental results. Table 3 gives the restricted list of configurations included in the scattering calculations to represent the target states.

3 Scattering calculation

The total wave function describing the (N+1)- electron system in an inner region $r \leq a$ is expanded on a discrete basis of R-matrix states [7,15].

$$\begin{aligned} \psi_k &= A \sum_{ij} C_{ijk} \Phi_i(x_1, x_2, ...x_N, r_{N+1}, \sigma_{N+1}) u_{ij}(r_{N+1}) \\ &+ \sum_j d_{jk} \phi_j(x_1.....x_{N+1}) \end{aligned} \tag{3}$$

where A is the antisymmetrization operator which accounts for electron exchange, and Φ_i channel function formed by coupling the target states of coordinates $x_i = \{r_i, \mathbf{r_i}, \sigma_i\}$ with the spin angle function of the scattered electron in order to form eigenstates of the total angular momentum J_t and parity π_t . More precisely, following Scott and Burke [8] the pair coupling scheme

$\mathbf{J} + \mathbf{l} = \mathbf{K}$, $\mathbf{K} + 1/2 = \mathbf{J_t}$

is used, since this coupling scheme is expected to be approximately realized in medium size atomic systems. The u_{ij} form a discrete R-matrix basis of continuum orbitals for the scattered electron and the $\{\phi_j\}$ are (N+1)-electron bound configurations, which account for the orthogonality of the continuum orbitals to the bound orbitals, and also for short range correlation effect.

The continuum orbitals u_{ij} in equation (3) are solutions of the radial differential equation,

$$[-\frac{d^2}{dr^2} + \frac{l_i(l_i+1)}{r^2} + 2V(r) - k_i^2] u_{ij}(r) = \sum_k \lambda_{ijk} P_{kl_i}(r) \tag{4}$$

which satisfy the boundary conditions,

$$u_{ij}(0) = 0 \tag{5}$$

$$\frac{a}{u_{ij}} \frac{du_{ij}}{dr}|_{r=a} = b \tag{6}$$

In equation (4), l_i is the angular momentum of the scattered electron, V(r) is the static potential of the target in its ground state and λ_{ijk} are the Lagrange mulipliers which are determined by imposing the othogonality of the continuum orbitals to the bound radial orbitals with the same value of l_i. We imposed a zero order logarithmic derivative at the R-matrix boundary $a = 2.20$

a.u. and we retained 12 continuum orbitals for each angular symmetry, to ensure convergence in the energy range considered here. The coefficients C_{ijk} and d_{jk} in equation (3) were determined by diagonalizing the (N+1)-electron Breit-Pauli Hamliltonian matrix in the inner region. In the outer region it is important to take account of long-range coupling between the channels. The resulting coupled equations are solved using a perturbation method developed by Seaton [16] to yield K matrix and then the collision strengths. In our calculations, we have considered all partial waves up to L=9 for both parities and spin multiplicities (Singlets and Triplets). This was sufficient to obtain convergent results for forbidden transitions from the ground and excited states. However for dipole allowed transitions, it was necessary to include the contribution of higher partial waves for convergence, using the extrapolation procedure described by Burke and Seaton [17].

4 Result and discussion

Figure 1 illustrates the results for the excitation from the ground state $1s^2\ 2s^2\ 2p^6\ ^1S^e$ to the first excited state $1s^2\ 2s^2\ 2p^5 3s\ ^3P^0_2$. It shows clearly, at low energies, the collision strengths are dominated by closed channel (or Feshbach) resonances. These resonances converge to threshold beyond the first excited state.

In table 4 our total collision strength at incident electron energies from 65 to 150 Ryd. are presented for all transitions within the first five fine structure levels corresponding to $1s^2\ 2s^2\ 2p^6\ ^1S^e$ and $1s^2\ 2s^2\ 2p^5\ 3s\ (^1P^0, ^3P^0)$ configurations of Ni XIX using Breit-Pauli approximation. As shown in table 4 among the transition from the ground state, the transition from 1 to 3 i.e. $^1S^e$ to $^1P^0$ transition have largest collision strength as it is dipole allowed (E1) transition and corresponds to excitation of electron from 2p state to 3s state. The collision strength for transition from 1 to 4 is smallest as it is spin forbidden and corresponds to $J_i = 0$ to $J_f = 0$ transition. For the transitions from the first excited state we find the collision strength for $^3P^o_2$ to $^3P^o_0$ (i.e 2 to 4) is lowest as it corresponds to electric quadrupole transition. Among the transitions from second excited state, the collision strength is larger for the intercombination transition $^1P^o_1$ to $^3P^o_1$ which corresponds to $\triangle J$ =0. The magnetic dipole transition from 4 to 5 i.e. $^3P^o_1$ to $^3P^o_1$ which is observed in solar flare by Feldmann et al [5] also has high collision strength. In table 5 we have compared our result with the calculation of Zhang et al [6]. Zhang et al [6] have reported the fine structure collision-strength for transitions from ground state of many neon-like ions including Ni XIX in the Coulomb-Born exchange method. For dipole allowed transition from the ground state i.e. $^1S^e_0$ to $^1P^o_1$ at E=77.85 Ryd. we have Ω_Z =1.88 and our result at this energy is Ω =1.878, two results are in quite close agreement. As can be seen from table 5, for spin forbidden transition 1 to 5 i.e. $^1S^e_0$ to $^3P^o_1$ at E=99.19 Ryd. we have Ω_Z =1.84 and our result is Ω = 1.883. There is reasonably good agreement among the two calculations.

In many astrophysical and plasma applications, the fine structure rate coefficients are needed and these are obtained by averaging total collision strengths over a Maxwellian distribution of electron energies. The excitation rate coefficients for a transition from state i to a state f at electron temperature T_e is given by

$$C(i \rightarrow f) \quad = \frac{8.63 \times 10^{-6}}{g_e T_e^{1/2}} \quad \gamma(i \rightarrow f) \quad exp(-\frac{\triangle E_{if}}{kT_e}) \quad cm^3 s^{-1} \tag{7}$$

where $g_i = (2j_i + 1)$ is the statistical weight of the lower level i, $\triangle E_{if} = E_f - E_i$ is the excitation energy, and $\gamma(i \rightarrow f)$ is the effective collision strength given by

$$\gamma(i \rightarrow f) = \int_0^\infty \Omega(i \rightarrow f) exp(-\frac{\epsilon_f}{kT_e}) \tag{8}$$

Here $\gamma(i \rightarrow f)$ is the total collision strength for transitions between level i and f, ϵ_f is the energy of incident electron with respect to the upper level f, T_e is the electron temperature, and k is the Boltzmann constant. In table 6 we have given $\gamma(i \rightarrow f)$ for 10 transitions from the ground state and first three excited states to fine structure levels of $1s^2 2s^2 2p^5 ({}^1P_1^0 \ , \quad {}^3P_{2,1,0}^0)$, from electron temperature $T_e = 0.5 \times 10^4$ to $T_e = 1.0 \times 10^5$ in ${}^0K$.

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Table 1: Parameters of the Radial functions of Ni XX

Orbitals	Power of r	Exp.	Coeff.
3s	1	20.60692	0.2312505
	2	8.98607	-1.1264039
	3	6.92923	1.6002710
3p	2	9.83896	2.3803094
	3	10.38145	-2.7699178
3d	3	13.18651	1.0000000
4d	3	14.11282	0.6332913
	4	7.81852	-1.1473076

Table 2: Excitation threshold for Ni XIX (in Ryd.)

Key	Level	State	J	Present	Experimental
1	$1s^2 2s^2 2p^6$	$^1S^e$	0	00.00000	00.00000
2	$1s^2 2s^2 2p^5 3s$	$^3P^0$	2	64.84234	64.73631
3	$1s^2 2s^2 2p^5 3s$	$^1P^0$	1	65.00092	64.89123
4	$1s^2 2s^2 2p^5 3s$	$^3P^0$	0	66.13064	
5	$1s^2 2s^2 2p^5 3s$	$^3P^0$	1	66.22816	66.13419

Table 3: Configuration used in the CI expansion of Ni XIX target states

State	Key	Configuration
$^1S^e$	1	$[1s^2]2s^2 2p^6$,$2s^2 2p^5 3p$,$2s^2 2p^5 4p$,$2s2p^6 3d$.
$^3P^0$	2,4,5	$[1s^2]2s^2 2p^5 3d$,$[1s^2]2s^2 2p^5 3s$,$[1s^2]2s^2 2p^5 4d$, $[1s^2]2s2p^6 3p$,$[1s^2]2s2p^6 4p$.
$^3P^0$	3	$[1s^2]2s^2 2p^5 3d$,$[1s^2]2s^2 2p^5 3s$,$[1s^2]2s^2 2p^5 4d$, $[1s^2]2s2p^6 3p$,$[1s^2]2s2p^6 4p$.

Table 4: Collision strengths Ω in Ni XIX in the energy range from 65 to 150 Ryd.

TRANSITIONS($i \rightarrow f$)	$1 \rightarrow 2$	$1 \rightarrow 3$	$1 \rightarrow 4$	$1 \rightarrow 5$	$2 \rightarrow 3$
E(in Ryd.)	Ω	Ω	Ω	Ω	Ω
65.00	1.475(-3)	-	-	-	-
70.00	1.405(-3)	1.607(-3)	2.977(-4)	1.421(-3)	5.200(-2)
80.00	1.328(-3)	1.932(-3)	3.729(-4)	1.520(-3)	4.989(-2)
90.00	1.218(-3)	2.150(-3)	2.272(-4)	1.877(-3)	3.477(-2)
100.00	1.029(-3)	2.215(-3)	2.145(-4)	1.961(-3)	3.022(-2)
110.00	8.365(-4)	2.332(-3)	1.630(-4)	2.071(-3)	2.435(-2)
120.00	7.859(-4)	2.589(-3)	1.599(-4)	2.142(-3)	2.109(-2)
130.00	7.039(-4)	2.697(-3)	1.412(-4)	2.224(-3)	1.922(-2)
140.00	6.785(-4)	2.847(-3)	1.297(-4)	2.330(-3)	1.795(-2)
150.00	5.361(-4)	3.359(-3)	1.037(-4)	2.344(-3)	1.679(-2)
TRANSITIONS($i \rightarrow f$)	$2 \rightarrow 4$	$2 \rightarrow 5$	$3 \rightarrow 4$	$3 \rightarrow 5$	$4 \rightarrow 5$
E(in Ryd.)	Ω	Ω	Ω	Ω	Ω
70.00	9.497(-3)	4.904(-2)	2.390(-2)	7.600(-2)	1.649(-2)
80.00	8.708(-3)	4.158(-2)	2.108(-2)	6.215(-2)	1.600(-2)
90.00	8.334(-3)	3.554(-2)	1.497(-2)	3.634(-2)	9.792(-3)
100.00	7.824(-3)	3.329(-2)	1.206(-2)	2.939(-2)	8.184(-3)
110.00	7.425(-3)	2.615(-2)	1.204(-2)	2.381(-2)	7.875(-3)
120.00	6.967(-3)	2.383(-2)	7.989(-3)	1.829(-2)	5.558(-3)
130.00	6.895(-3)	2.222(-2)	6.910(-3)	1.630(-2)	4.860(-3)
140.00	6.867(-3)	2.120(-2)	6.155(-3)	1.505(-2)	4.411(-3)
150.00	6.456(-3)	2.100(-2)	5.083(-3)	1.381(-2)	2.344(-3)

Table 5: Comparison of fine structure collision strengths obtained by Zhang et al (Ω_Z) with our results(Ω)

TRANSITIONS($i \rightarrow f$)	$1 \rightarrow 2$	$1 \rightarrow 2$	-	$1 \rightarrow 3$	$1 \rightarrow 3$
E(Ryd.)	Ω	Ω_Z	E(Ryd.)	Ω	Ω_Z
77.67	1.334(-3)	1.13(-3)	77.85	1.878(-3)	1.88(-3)
97.09	1.104(-3)	9.04(-4)	97.31	2.171(-3)	2.28(-3)
122.98	7.711(-4)	6.90(-4)	123.26	2.619(-3)	2.85(-3)
161.82	4.648(-4)	4.84(-4)	161.82	3.712(-3)	3.70(-3)
TRANSITIONS($i \rightarrow f$)	$1 \rightarrow 4$	$1 \rightarrow 4$	-	$1 \rightarrow 5$	$1 \rightarrow 5$
E(Ryd.)	Ω	Ω_Z	E(Ryd.)	Ω	Ω_Z
79.29	2.872(-4)	2.27(-4)	79.35	1.489(-3)	1.56(-3)
99.06	2.170(-4)	1.87(-4)	99.19	1.883(-3)	1.84(-3)
125.64	1.570(-4)	1.38(-4)	125.64	2.166(-3)	2.25(-3)
165.09	9.097(-5)	9.68(-5)	165.31	2.862(-3)	2.87(-3)

Table 6: Effective collision strength $\gamma(i \rightarrow f)$ for forbidden and allowed transitions in Ni XIX

TRANSITIONS$(i \rightarrow f)$	$1 \rightarrow 2$	$1 \rightarrow 3$	$1 \rightarrow 4$	$1 \rightarrow 5$	$2 \rightarrow 3$
E$(i \rightarrow f)$(in e.v)	0.8822(+3)	0.8843(+3)	0.8997(+3)	0.9010(+3)	0.2158(+1)
TEMP(^0K)	γ	γ	γ	γ	γ
0.5000(+4)	0.3729(-2)	0.1558(-2)	0.3103(-3)	0.1370(-2)	0.6308(-1)
0.7500(+4)	0.2604(-2)	0.1572(-2)	0.3049(-3)	0.1364(-2)	0.6267(-1)
0.1000(+5)	0.2122(-2)	0.1585(-2)	0.3035(-3)	0.1362(-2)	0.6250(-1)
0.1500(+5)	0.1748(-2)	0.1603(-2)	0.3036(-3)	0.1361(-2)	0.6235(-1)
0.2000(+5)	0.1619(-2)	0.1615(-2)	0.3045(-3)	0.1361(-2)	0.6225(-1)
0.2500(+5)	0.1563(-2)	0.1624(-2)	0.3052(-3)	0.1361(-2)	0.6215(-1)
0.3000(+5)	0.1535(-2)	0.1632(-2)	0.3059(-3)	0.1362(-2)	0.6204(-1)
0.3500(+5)	0.1520(-2)	0.1638(-2)	0.3064(-3)	0.1362(-2)	0.6193(-1)
0.4000(+5)	0.1510(-2)	0.1644(-2)	0.3068(-3)	0.1362(-2)	0.6182(-1)
0.4500(+5)	0.1504(-2)	0.1649(-2)	0.3071(-3)	0.1363(-2)	0.6172(-1)
0.5000(+5)	0.1500(-2)	0.1654(-2)	0.3073(-3)	0.1363(-2)	0.6162(-1)
0.6000(+5)	0.1495(-2)	0.1661(-2)	0.3076(-3)	0.1365(-2)	0.6142(-1)
0.7000(+5)	0.1492(-2)	0.1666(-2)	0.3078(-3)	0.1366(-2)	0.6124(-1)
0.8000(+5)	0.1489(-2)	0.1668(-2)	0.3079(-3)	0.1367(-2)	0.6107(-1)
0.9000(+5)	0.1488(-2)	0.1670(-2)	0.3079(-3)	0.1368(-2)	0.6090(-1)
0.1000(+6)	0.1486(-2)	0.1670(-2)	0.3079(-3)	0.1369(-2)	0.6074(-1)
TRANSITIONS$(i \rightarrow f)$	$2 \rightarrow 4$	$2 \rightarrow 5$	$3 \rightarrow 4$	$3 \rightarrow 5$	$4 \rightarrow 5$
E$(i \rightarrow f)$(in e.v)	0.1753(+2)	0.1886(+2)	0.1537(+2)	0.1670(+2)	0.1328(+1)
TEMP(^0K)	γ	γ	γ	γ	γ
0.5000(+4)	0.1018(-1)	0.5409(-1)	0.2965(-1)	0.9128(-1)	0.1932(-1)
0.7500(+4)	0.1016(-1)	0.5382(-1)	0.2876(-1)	0.9080(-1)	0.1922(-1)
0.1000(+5)	0.1014(-1)	0.5372(-1)	0.2828(-1)	0.9059(-1)	0.1918(-1)
0.1500(+5)	0.1011(-1)	0.5362(-1)	0.2776(-1)	0.9035(-1)	0.1913(-1)
0.2000(+5)	0.1008(-1)	0.5356(-1)	0.2748(-1)	0.9018(-1)	0.1910(-1)
0.2500(+5)	0.1006(-1)	0.5351(-1)	0.2731(-1)	0.9003(-1)	0.1907(-1)
0.3000(+5)	0.1004(-1)	0.5346(-1)	0.2718(-1)	0.8989(-1)	0.1904(-1)
0.3500(+5)	0.1003(-1)	0.5342(-1)	0.2708(-1)	0.8975(-1)	0.1902(-1)
0.4000(+5)	0.1001(-1)	0.5338(-1)	0.2700(-1)	0.8961(-1)	0.1899(-1)
0.4500(+5)	0.1000(-1)	0.5333(-1)	0.2693(-1)	0.8948(-1)	0.1897(-1)
0.5000(+5)	0.9992(-2)	0.5329(-1)	0.2687(-1)	0.8934(-1)	0.1894(-1)
0.6000(+5)	0.9974(-2)	0.5321(-1)	0.2677(-1)	0.8908(-1)	0.1889(-1)
0.7000(+5)	0.9958(-2)	0.5313(-1)	0.2669(-1)	0.8882(-1)	0.1885(-1)
0.8000(+5)	0.9944(-2)	0.5305(-1)	0.2661(-1)	0.8856(-1)	0.1880(-1)
0.9000(+5)	0.9932(-2)	0.5297(-1)	0.2654(-1)	0.8830(-1)	0.1875(-1)
0.1000(+6)	0.9920(-2)	0.5289(-1)	0.2647(-1)	0.8804(-1)	0.1870(-1)

Figure 1: Total collision strength for the transition $1s^2\ 2s^2\ 2p^6\ {}^1S^6 \rightarrow 1s^2\ 2s^2\ 2p^5\ 3s\ {}^3P_2^o$ in Ni XIX as a function of electron energy in Rydberg.